# Phase transition of Sr on Si (0 0 1): First principles prediction and experiment

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Understanding and predicting temperature dependent surface phases from first principles can be invaluable in developing and optimizing processes for the growth of epitaxial structures. In particular, an ordered sub-monolayer phase of Sr on Si (001) plays a key role in determining the quality of the interface in the most commonly used method for growing epitaxial oxides on Si. Using density functional theory, we build a first principles model of sub-monolayer Sr on Si, which we use to determine the temperature dependent phase equilibrium between an ordered 1/6 ML structure and a disordered lattice gas. In addition, we experimentally determine this phase diagram using RHEED and find quantitative agreement between theoretical predictions and experiment.